CONSISTENT TRANSPORT THEORY OF PARTICLES AND RADIATION

I. THE BASIC FORMULATION

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ABSTRACT

We expose a consistent theory for dealing with transport phenomena in many astrophysical conditions. The present paper gives a more general frame to the classical radiative transfer theory and some particle transport phenomena. We start with the kinetic equations and introduce three cases: LTE, partial LTE (usually called non-LTE), and non-LTE (or fully non-LTE).

We present the fully consistent equations for partial LTE, and define the transport coefficients (which also hold for LTE) and show a method for calculating these coefficients as well as their validity range. The method is based on a numerical solution of the kinetic equations considering Landau, Boltzmann and Focker-Planck collision terms.

I. Introduction

Radiation transport has been thoroughly treated since the beginning of astrophysical research, as can be seen in, e.g., Athay (1972) and Mihalas (1978), but as a subject independent of matter transport and assuming that particles follow a Maxwellian distribution.

On the other hand particle transport phenomena have been studied without considering the radiation. Two different situations have been considered, the first corresponds to cases where particle distribution functions are very close to Maxwell's function and the second to the case where non-local effects dominate the distributions.

The particle transport for small departures from Maxwellian distribution has been analyzed by several authors. The early work by Chapman, Enskog and Burnett (hereafter CHEB) as discussed by Chapman and Cowling (1936, hereafter CC), led to a complete compilation of transport coefficients, definitions and calculation methods very usefull for atomic and molecular gases. Their approach is based on expansion of the distribution functions in the vicinity of the Maxwell distribution function, then, they retain only the first term in that expansion and in turn expand again that first order term f^1 in Laguerre polinomials up to some order N. An application of the CC methods to mixtures of gases without considering radiation, is due to Devoto (1966).

The CHEB method has also been applied to ionized gases, by Braginskii (1965), but that case requires expansions up to at least second order (N=2). The CHEB method was also aplied by Hochestim (1967) to magnetized plasmas by using expansion up to order 20.

As an alternative method for calculating the first order departure from Maxwellian distribution, Spitzer and Harm (1953, hereafter SH) have calculated, (in the case of a gas composed of electrons and one ionic species), not only the transport coefficients, but also the detailed shape of the distributions function, by a numerical method without restrictions to a truncated polynomial expansion.

The results by SH have been used extensively in several fields of physics and also show the limits of validity of the first order distribution function approach. Those results led to the analytical approach of Shvarts et al. (1981) for calculating flux limit coefficients which have been qualitatively confirmed by experiments. Also an analytical approach was applied by Campbell (1984) for very simplified cases.

An approach which fits the capabilities of modern "supercomputers" has been suggested by Fontenla (1985) showing how one can define a set of transport coefficients and calculate them by numerical methods. A similar method has been used by Epperlein and Haines (1986) for a fully ionized gas with magnetic field.

We also mention papers relating to particle transport case where non-local effects are very important. In that cathegory the paper by Luciani, Mora and Pellat (1985) assumes a very simplified kinetic equation and presents an approach to some nonlocalized heat flux which arises when the transport becomes non-local. Calculations of non-local effects have likewise been carried out by Roussell-Dupree (1980), Shoub (1983) and by Owocki and Canfield (1986) for the solar transition region.

In the present paper we show the full set of kinetic equations which have to be considered for a consistent treatement of both radiation and particle transport phenomena. From these equations we derive a set of hydrodynamic equations for particles without any apriori assumption regarding the radiation field or the distribution functions.

We characterize some different regimes and also define and explain the definitions of some transport coefficients. The basis of the numerical method for calculating these transport coefficients is explained. Then, we show some results in a simple case and compare with the previously mentioned papers.

II. The Kinetic Equations

Following the Ehler and Kohler (1977) formalism, and assuming that all the requirements related to statistics are satisfied, we describe the macroscopic system by the one particle distribution function for each of the present species (α).

We consider the phase space composed of the four dimensional coordinates (x,y,z,ict) and the four dimensional momenta $\vec{P}$ $(p_x, p_y, p_z, iE/c)$ where i is the imaginary numbers unit, c the velocity of light, E the total energy; and the other variables have the usual meaning. For a particle of rest mass m, $|\vec{P}| = imc$ and for photons $|\vec{P}| = 0$. Hence, the impulse have only three independent variables.

Following Ehler and Kohler we write the volume measure in orbital phase for particles of given rest mass

$$d\omega' = (\vec{P} \cdot d\vec{\sigma})\, d\pi', \tag{1}$$

where $d\vec{\sigma}$ is an space-time surface element, and $d\pi'$ the volume element in four momentum space for that particle. Then,

$$d\pi' = \frac{dp_x\, dp_y\, dp_z}{E/c} \tag{2}$$

We have assumed a gas of particles which are essentially free; i.e., interactions between them are short-lived compared to the time between such interactions (small range interactions). The particles are subject to a general field which can include the autoconsistent field. In the case of plasmas, there is also some permanent interaction between particles, but to the extent this is small compared to the kinetic energy of the particles, it only affects the spatial dependence of the distribution function (leading to Debye screening) and then does not affect the present work (for more details see e.g., Balescu, 1975).

According to our definitions and assuming summation over repeated indices, we have the definition of the distribution function f' according to

$$N_{\Sigma} = \int_{\Sigma,\infty} f'd\omega' = \int_{\Sigma} d\vec{\sigma} \cdot \left(\int_{\infty} \vec{p}\, f'\, d\pi'\right) = \int_{\Sigma} \vec{j} \cdot d\vec{\sigma} \, , \qquad (3)$$

where the integral over ∞ means integration over the whole momentum space, N being the number of particle trajectories which cross the surface Σ, and $\vec{j}$ the four-vector current density of the species. Then if n_{α} is the volume density of the species α

$$j_{4\alpha} = i \int_{\infty} \frac{E}{c} f'_{\alpha}\, d\pi'_{\alpha} = in_{\alpha} \, . \qquad (4)$$

Redefining f' and $d\pi'$ in order to work with the state occupation numbers and the state densities, we write

$$f = \frac{h^3}{w} f' ; \; d\pi = \frac{w}{h^3} d\pi' ; \; d\pi^* = \frac{E}{c} d\pi \, , \qquad (5)$$

resulting in

$$n_{\alpha} = \int f_{\alpha} d\pi_{\alpha}^*$$

where w is the multiplicity of the state, and h Planck's constant; Then,

$$\text{for particles} \qquad d\pi^* = (2S+1)\left(\frac{mc}{h}\right)^3 \gamma^5\beta^2 d\beta d\mu d\phi \ ,$$

$$\text{and for photons} \qquad d\pi^* = 2\left(\frac{\nu_o}{c}\right)^3\left(\frac{\nu}{\nu_o}\right)^2 d\left(\frac{\nu}{\nu_o}\right) d\mu d\phi \ , \tag{6}$$

where S is the spin, β the velocity in units of the velocity of light, γ the relativistic correction $\gamma = (1 - \beta^2)^{-1/2}$ and θ and ϕ the spherical angles which define the direction of the vector $\vec{p}$ in the three dimensional space; $\mu = \cos\theta$ is the projection factor along the z axis and ν the photon frequency. The quantity ν_o represents an arbitrary frequency taken to dimensionalize the variable.

The force is assumed to include gravitational and Lorentz terms

$$\frac{\vec{F}}{c} = \left[\frac{m}{c}\vec{g} + \frac{Ze}{c}\vec{E} + \frac{Ze}{mc^2\gamma}(\vec{P}\cdot\vec{B})\right] \ , \tag{7}$$

where $\vec{g}$ is the gravitational acceleration, $\vec{E}$ and $\vec{B}$ the electric and magnetic fields,respectively, e the proton charge and Z the charge of particle in units of e.

The Liouville equations (see Ehlers and Kohler 1977) take the form in the case of special relativity for particles

$$\beta\, n_i \frac{\partial f}{\partial x_i} + \frac{1}{c}\frac{\partial f}{\partial t} + \frac{F_i}{c}\cdot\frac{\partial f}{\partial p_i} = \frac{\zeta}{mc\gamma} = \xi$$

and for photons

$$n_i \frac{\partial f}{\partial x_i} + \frac{1}{c}\frac{\partial f}{\partial t} = \frac{\zeta}{\frac{h\nu}{c}} = \xi \ , \qquad (9)$$

where $\vec{n}$ indicates the unit vector in the direction of the impulse and n_i its components, ξ is the collision density for the particles considered (ζ is the invariant collision density) and we use (as in the following) the convention of summation over repeated indices.

Equation (9) applies to cases where the space and time variations of the distribution functions are negligible through the range of the forces between particles responsibile of the collision terms. Another condition required in this approach is that all fields ($\vec{g}$, $\vec{E}$ and $\vec{B}$) are small enough not to affect the collisions, i.e., they do not produce any noticeable change in particle impulse during the duration of a collision.

We remark that the collision densities just mentioned are the sum of all the collision terms between a particle within one phase space cell (according to the quantum mechanical definition of states) with all other particles, even those of the same species. Then these collision densities are integral nonlinear functions of the distribution functions.

Considering the terms which can be expressed in the Boltzmann form, for a species with a certain value of the impulse (within a cell of phase space), namely A, they can be expresed as a source term which does not depend on f_A, but depends on the other particle (or photon) distribution functions f_B, f_C, etc., and a sink term which is proportional to f_A, so that

$$\xi_A = \eta_A - \chi_A f_A \ . \tag{10}$$

Following Ehlers and Kohler, we adopt the definitions

$$f^A = 1 + f_A \qquad \text{for bosons}$$
(11)
$$f^A = 1 - f_A \qquad \text{for fermions.}$$

Then, for collisions between a particle A and a particle B, which result in the emission of particles C and D (binary collisions), where $d\sigma = \sigma\ d\mu\ d\phi$, is the differential cross-section in the inertial frame, we have

$$\eta_A = \iint f_C f_D\ f^B\ \beta_{AB}\ d\sigma\ d\pi_B{}^* \ ,$$
(12)
and $$\chi_A = \iint f_B f^C f^D\ \beta_{AB}\ d\sigma\ d\pi_B{}^* \pm \eta_A \ .$$

The minus sign holds when A's are bosons, and the plus sign when they are fermions. The expression for β_{AB} is derived from Ehlers and Kohler's definition of P_{AB}, i.e.

$$\beta_{AB} = (\beta_A{}^2 + \beta_B{}^2 - 2\beta_A\beta_B \cos\ \theta_{AB} - \beta_A{}^2\beta_B{}^2 \sin^2\theta_{AB})^{1/2} , \tag{13}$$

where θ_{AB} is the angle between $\vec{p}_A$ and $\vec{p}_B$. This expression is also valid when one of the particles is a photon, in which case the corresponding β_{AB} will be unity.

For the conditions prevailing in many astrophysical situations degeneracy is negligible and $f^A = 1$ for particles. This simplifies slightly some equations, and if required, the equations below can be modified to account for degeneracy.

The above considerations regarding Boltzmann collision terms hold for both elastic and inelastic collisions. Boltzmann type terms can also account for collisions involving many incident and/or resultant particles or photons, as for instance collisional ionization and recombination.

In the case of elastic, binary collisions, if only small changes in the particles impulses occur after the collision, the Boltzmann term is not suitable for numerical calculations, since it involves a large extent of numerical cancellation between the source and sink terms.

For instance, when a particle A undergoes a collision with a much lighter particle B or with a photon of moderate frequency (frequency much smaller than the Compton frequency) the impulse of particle A changes by only a small amount. The source and sink terms in the Boltzmann term can be expanded and we obtain the Focker-Planck collision term (see Balescu 1975), viz.

$$\xi_A = \frac{\partial}{\partial P_{A_i}} \left(- \langle \Delta p_i \rangle f_A + \langle \Delta P_i \Delta P_j \rangle \frac{\partial f_A}{\partial P_j}\right) \qquad (14)$$

where

$$\langle \Delta P_i \rangle = - \frac{v_i}{v} m_A c \int \beta^2_{AB} \, D \, f_B \, dp_B{}^* \, ,$$

$$\langle \Delta P_i \Delta P_j \rangle = m^2{}_A c^2 \int \beta^3_{AB} \left[A \, \delta_{ij} + (B - A) \frac{\beta_{AB_i} \beta_{AB_j}}{\beta^2_{AB}}\right] f_B d\pi_B{}^* \, ,$$

and the coefficients D, A, and B are given by the expressions:

$$D = \int (1 - \mu')\sigma' d\mu' d\phi' \ ,$$

$$A = \frac{1}{2} \int (1 - \mu'^2)\ \sigma' d\mu' d\phi' \ ,$$

$$B = \int (1 - \mu')^2\ \sigma' d\mu' d\phi' \ .$$

Here $\sigma' d\mu' d\phi'$ is the differential cross section in the center of mass coordinate system (if one of the species is a photon, the rest frame of the particle is the reference system), and δ_{ij} is the Kronecker delta.

The case of charged particles involves collisions where not only the impulse of particle A but also that of particle B changes slightly as a result of the collision. This case is particularly important for Coulomb type forces since for them the cross-section diverges when the deviation angle goes to zero, and this kind of collisions dominate in normal plasmas.

For Coulomb collisions we use the Landau (1936) form of the Focker-Planck collision term as shown in Balescu (1975), i.e.

$$\xi_A = \int \frac{\partial}{\partial P_{Ai}} \left[G_{ij}\left(\frac{\partial f_A}{\partial P_{Aj}} f_B - \frac{\partial f_B}{\partial P_{Bj}} f_A\right)\right] d\pi_B{}^* \ , \tag{15}$$

with

$$G_{ij} = m_A^2 c^2 \left[A\delta_{ij} + (B-A) \frac{\beta_{AB_i} \beta_{AB_j}}{\beta_{AB}^2}\right] . \tag{16}$$

The expression for derivatives with respect to the components of impulse can be obtained from the expression

$$mc\frac{\partial}{\partial p_i} = \frac{n_i}{\gamma^3}\frac{\partial}{\partial\beta} + \frac{(\delta_{iz} - \mu n_i)}{\gamma\beta}\frac{\partial}{\partial\mu} + \frac{(n_y\delta_{ix} - n_x\delta_{iy})}{\gamma\beta(1-\mu^2)} \cdot \frac{\partial}{\partial\phi} , \qquad (17)$$

where δ_{ij} is the Kronecker delta and n_i are the components of the unit vector $\vec{n}$ in the direction of $\vec{p}$.

By including the explicit formula for the collision terms we find

$$\beta\, n_i \frac{\partial f}{\partial x_i} + \frac{1}{c}\frac{\partial f}{\partial t} + \frac{F_i}{c}\frac{\partial f}{\partial p_i} = \eta + Df - \chi f - \phi_i \frac{\partial f}{\partial p_i} , \qquad (18)$$

where

$$Df = \psi_{ij}\frac{\partial^2 f}{\partial p_i \partial p_j} ,$$

$$\eta = \sum_B \eta ,$$

$$\chi = \sum_B \left[\chi + \frac{\partial\langle\Delta P_j\rangle}{\partial P_j} + \int \frac{\partial G_{j\beta}}{\partial P_j}\frac{\partial f_B}{\partial P_{B_\beta}} d\pi_B{*}\right] ,$$

$$\phi_i = \sum_B \left[\langle\Delta P_i\rangle - \frac{1}{2}\frac{\partial\langle\Delta P_i \Delta P_j\rangle}{\partial p_j} + \int G_{ij}\frac{\partial f_B}{\partial P_{B_j}} d\pi_B^* - \int \frac{\partial G_{ij}}{\partial P_j} f_B d\pi_B^*\right],$$

and $\psi_{ij} = \sum_B \left[\frac{\langle\Delta P_i \Delta P_j\rangle}{2} + \int G_{ij} f_B d\pi_B^*\right]$.

These equations describe the transport of particles and radiation and take into account the full interaction between matter and radiation in astrophysical problems, dealing with medium density gases like the ones that form the stellar atmospheres.

One of these equations can be simplified for problems where the photon flight time over a characteristic length is small compared to the characteristic times for variations of physical parameters. In the latter case one can neglect the accumulation of photons in regions of space and drop the term $(1/c)((\partial f/\partial t)$, recovering the ususal radiation transport equation (Athay, 1972).

The basic kinetic equations can also be obtained from the BBGKY chain of equations by applying statistical assumptions (see Balescu 1975).

III. The Hydrodynamic Equations

These equations can be derived from the moments of the kinetic equations (18) considering only particles (i.e., excluding radiation), and differ from some others which include radiation in the moments of the kinetic equations (see for example Anderson, 1976). The reason for the present formulation lies in the fact that for most cases in stellar atmospheres the radiation spectrum has to be solved in detail, and its agreement with observations is the main goal.

We define the moments of the collision term ξ_α for the α particles by

$$R_\alpha = \int \xi_\alpha d\pi_\alpha ; \quad \vec{P}_\alpha = \int m_\alpha \vec{v} \xi_\alpha d\pi_\alpha ; \quad \varepsilon_\alpha = \int m_\alpha \frac{v^2}{2} \xi_\alpha d\pi_\alpha , \tag{20}$$

where $d\pi_\alpha$ is the impulse phase-space volume element, m_α is the mass of particles of species α, and $\vec{v}$ is the velocity.

With these definitions, the statistical equilibrium equations become

$$\frac{\partial n_\alpha}{\partial t} + \nabla \cdot (n_\alpha \vec{V}_\alpha) + \nabla \cdot (n_\alpha \vec{U}) = R_\alpha , \tag{21}$$

where n_α is the number density of α particles, $\vec{V}_\alpha$ their diffusion velocity, $\vec{U}$ the fluid velocity (mass center velocity), and R_α is the net rate of creation of α particles per volume unit.

Since mass is conserved in all collisions, the usual mass conservation equation holds, i.e.

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\vec{U}) = 0, \tag{22}$$

where ρ is the mass density.

Taking the first moment of the kinetic equations we find

$$\frac{\partial(\rho\vec{U})}{\partial t} + \nabla\cdot(\overline{\overline{\pi}}) = \vec{F} + \vec{\mathcal{P}} , \tag{23}$$

where

$$F = \sum_{\alpha} \rho_\alpha \vec{a}_\alpha , \quad \vec{\mathcal{P}} = \sum_{\alpha} \vec{\mathcal{P}}_\alpha , \quad \rho_\alpha = n_\alpha m_\alpha ,$$

and $\vec{a}_\alpha$ is the acceleration experinced by an α particle due to all external (or autoconsistent) fields. $\vec{\mathcal{P}}$ is the net gain of particle impulse per volume unit due to inelastic collisions with photons. The last quantity equals the net loss of photon impulse and can be expressed in terms of the collisional term for radiation

$$\vec{\mathcal{P}} = \frac{1}{c}\int(\kappa_\nu I_\nu - \varepsilon_\nu)\ \vec{n}\ d\omega\ d\nu, \tag{24}$$

where c is the speed of light, κ_ν, I_ν, and ε_ν have their usual meaning of absorption coefficient, intensity and emissivity of radiation at frequency ν and with direction $\vec{n}$, and $d\omega$ is the solid angle element.

As mentioned before, when the photon flight time over a characteristic length is small, the kinetic equation for photons gives

$$\vec{P} = \frac{1}{c}\, \nabla \cdot \int \vec{n}\, \vec{n}\, I_\nu \, d\omega \, d\nu \,, \tag{25}$$

where $\frac{1}{c} \int \vec{n}\, \vec{n}\, I_\nu \, d\omega \, d\nu$ the radiation pressure tensor.

The tensor $\bar{\bar{\pi}}$ contains the pressure p, the viscous stress $\bar{\Gamma}$ (of null trace), and the terms due to diffusion, viz.

$$\bar{\bar{\pi}} = p\, \bar{I} + \bar{\bar{\Gamma}} + \sum_\alpha \rho_\alpha \vec{V}_\alpha \vec{V}_\alpha , \tag{26}$$

where

$$p = \sum_\alpha p_\alpha ,\; p_\alpha = \frac{1}{3}\, \mathrm{Tr} \int m_\alpha \vec{w}\, \vec{w}\, f_\alpha d\pi_\alpha ;$$

and
$$\bar{\bar{\Gamma}} = \sum_\alpha \bar{\bar{\Gamma}}_\alpha ;\; \bar{\bar{\Gamma}}_\alpha = \int m_\alpha \vec{w}\vec{w} f_\alpha d\pi_\alpha - p\bar{I} \,,$$

with the definition $\vec{w} = \vec{v} - (\vec{U} + \vec{V}_\alpha)$. In equation (26) many authors drop the last term because it is quadratic in V_α.

The kinetic energy equation for the gas is

$$\frac{\partial}{\partial t}\left(\frac{3}{2}\, p + \sum_\alpha \rho_\alpha \frac{V_\alpha^2}{2}\right) + \nabla \cdot \left[\vec{U}\left(\frac{3}{2}\, p + \sum_\alpha \rho_\alpha \frac{V_\alpha^2}{2}\right)\right] +$$

$$+ \nabla \cdot \left[\sum_\alpha \vec{V}_\alpha \left(\frac{3}{2}\, p_\alpha + \rho_\alpha \frac{V_\alpha^2}{2}\right)\right] + (\bar{\bar{\pi}} \cdot \nabla) \cdot \vec{U} + \nabla \cdot \left(\sum_\alpha \bar{\bar{\pi}}_\alpha \cdot \vec{V}_\alpha\right) + \tag{27}$$

$$+ \nabla \cdot \vec{q} = \sum_\alpha \rho_\alpha \vec{a}_\alpha \cdot \vec{V}_\alpha + \varepsilon - \vec{U} \cdot \vec{P},$$

with $\varepsilon = \sum_\alpha \varepsilon_\alpha$, $\vec{q} = \sum_\alpha \vec{q}_\alpha$ and where $\vec{q}_\alpha$ is the conductive energy flux for α particles, given by

$$\vec{q}_\alpha = \int \vec{w}\, m_\alpha \frac{w^2}{2} f_\alpha\, d\pi_\alpha . \tag{28}$$

This definition of conductive flux agrees with the one from CC since it does not contain the thermal energy flux due to diffusion

$$\sum_\alpha \left[\vec{V}_\alpha\left(\frac{3}{2} p_\alpha + \rho_\alpha \frac{V_\alpha^2}{2}\right) + \bar{\bar{\pi}}_\alpha \cdot \vec{V}_\alpha\right] , \tag{29}$$

or $\sum_\alpha \vec{V}_\alpha \frac{5}{2} p_\alpha$ up to first order in $\vec{V}_\alpha$ and $\bar{\bar{\Gamma}}$.

The term $\vec{U} \cdot \vec{P}$ is frequently dropped for non-relativistic cases. Again, the condition for energy balance in collisions gives

$$\sum_\alpha (\varepsilon_\alpha + R_\alpha E_\alpha) = \int (\kappa_\nu I_\nu - \varepsilon_\nu)\, d\omega\, d\nu, \tag{30}$$

where E_α is the internal energy per α particle.

There results then

$$\varepsilon = - \sum_\alpha E_\alpha\left[\frac{\partial n_\alpha}{\partial t} + \nabla\cdot(n_\alpha \vec{V}_\alpha) + \nabla\cdot(n_\alpha \vec{U})\right] + \int (\kappa_\nu I_\nu - \varepsilon_\nu)\, d\omega\, d\nu .$$

By using the previous equations one can easily transform the thermal energy equation into the entalpy equation.

IV. Different Regimes

In principle, the system of eqs. (18) (in the following referred to as KE) must be solved simultaneously for all particles and radiation with specific boundary and initial conditions which define the problem under consideration. Furthermore, these equations have to be complemented with Maxwell's and gravitational field equations.

An inspection of the KE formulas shows that their right hand member (hereafter RHM) contains only local terms; i.e., the terms in RHM depend only on the values of the distribution functions at the specific space-time coordinates, and the terms in the left hand member (hereafter LHM) depend on the values of the distribution functions at other space-time coordinates (non-local).

The latter terms lead to the definition of the local thermodynamic equilibrium regime (LTE). This is, when the absolute value of all the terms in the LHM of all the KE equations are much smaller than the absolute value of the dominant terms in the corresponding RHM. In LTE situation, then, there is a strong cancellation between RHM terms, and the distributions become mainly locally defined by some thermodynamic equilibrium functions F (those which null the RHM) of some thermodynamic parameters (TP).

One complete set of TP is given by $(n, \vec{U}, T, A)$ where n is the total particle density, $\vec{U}$ the fluid velocity, T the temperature, and A the set of independent abundances of the species.

The case of LTE without considering radiation is analyzed in many text books which define the hydrodynamic equations (the equations which define the TP values as functions of space-time coordinates). In particular, Chapman and Cowling (CC) show the definitions of some transport coefficients and a method for calculating them. The case of a gas including radiation has been treated by Anderson (1976) showing some transport coefficients for a very simplified case.

On the other hand, when in all KE eqs. the RHM terms are at most of the order of magnitude of the LHM terms, we have what we call non-LTE (or fully non-LTE). In this case one has to use different approaches for solving the KE eqs. (e.g., Rousell-Dupree (1980), Shoub (1983) and Owocki and Canfield (1986). In non-LTE cases one can use the hydrodynamic equations (20) to (30) and define the parameters $\vec{U}$, p and T, but they do not have the general meaning they have in LTE, and they are useful only for correcting and checking consistency and errors in numerical methods.

In the non-LTE case the shape of the distribution functions is defined mainly by the boundary and initial conditions (i.e. non-locally defined).

Between the two extreme cases there is a wide range of intermediate cases, which cannot be treated like in LTE, but are far easier to solve than the non-LTE cases. This range has been considered for instance by Braginskii (1965) who showed that sometimes the shape of the distribution functions for different species can be close to the equilibrium function, but with different values of the TP for each species. This situation has also been considered by Nakagawa and Wu (1968) who included radiation.

We shall define a special case in this intermediate range and call it partial thermodynamic equilibrtium (p-LTE). Our definition results from considering the elastic collision terms in the KE eqs. for certain particles. If these terms are much larger than the corresponding terms in the LHM and RHM, the distribution functions for these particles (thermal particles) are close to some equilibrium functions. We can then take the moments of KE eqs. ,integrate them and perform the summation over the different species leading to the hydrodynamic equations described in eqs. (20) to (30). The latter equations in conjuction with the KE eqs. for the particles not included in the former (non-thermal particles) and photons constitute a complete set of equations (if the transport terms ($\vec{V}_\alpha$, $\bar{\bar{T}}$, $\vec{q}$) in the hydrodynamic equations are known).

We want to stress that while all particle species have elastic collisions with the same and other species, photons do not interact with themselves and their relaxation towards the equilibrium distribution function (or thermalization) is due to photon-particle interactions (which are inelastic collisions).

In many astrophysical situations the collision terms in the photons kinetic equations are not much larger than the corresponding LHM terms. Moreover, frequently in eqs. KE for particles, the order of magnitude of the LHM terms lies between those of elastic collisions (usually the largest) and inelastic collisions (the latter being the responsible for relaxation towards Saha-Botzmann equilibrium).

The former constitutes a typical p-LTE case, where one can assume that the shape of particle distribution functions are close to Maxwellian, due to the strong cancellation of elastic collisions terms. However, the species densities do not follow the Saha-Boltzmann formula and the radiation do not follow the Planck formula.

We write for the thermal particles

$$f_\alpha \approx M_\alpha = \frac{n_\alpha}{K} \{\pm 1 + \exp[\frac{mc^2(\gamma' - 1) - F_i x_i + E_\alpha}{kT}]\}^{-1}, \quad (31)$$

where k is the Boltzmann constant, K a normalization factor, and γ' the Lorentz factor in the fluid frame (with velocity $\vec{U}$). The minus sign holds for bosons, and the plus sign for fermions.

One additional advantage of the p-LTE formulation is that even the equations which one cannot include in the hydrodynamical eqs., become simpler, since in their RHM the larger terms are more or less simple functions of the TP instead of complicated nonlinear integrals. An example is the radiation transport equations, where the source term (photon emissivity) and the sink term (absorption coefficient) assume relatively simple expressions.

V. The Transport Coefficients

Some terms which appear in the hydrodynamic equations (20) thru (30) are related to the fluxes of particles and particle impulses and energies ($n_\alpha \vec{V}_\alpha$, $\bar{\bar{\Gamma}}_\alpha$, $\vec{q}_\alpha$) in the fluid rest frame.

These terms, as their definitions show, arise due to the anisotropy of the distribution functions. In the p-LTE case, for the thermal particles the fluxes are produced by the departure of the distribution functions from a maxwellian shape. Those departures (δf) are complicated functions of the LHM of the KE eqs. for the thermal particles, and the collisions with the non-thermal particles and photons. The moments of the functions δf or the terms ($\vec{V}_\alpha$, $\bar{\bar{\Gamma}}_\alpha$, $\vec{q}_\alpha$) can be tabulated for different conditions and interpolated for solving the actual problems.

We attempt to show a general method for calculating δf in p-LTE situations by using an iterative numerical scheme. The method consists in the application of the multidimensional Newton-Raphson numerical technique (hereafter NR) to the KE. We also suggest that this method might be applied for solving some non-LTE problems, since in many cases this method is successful in calculating the solutions of non-linear equations. However, the convergence of the method is not assured in general, and the method should be explored further to show its possible usefulness in solving KE eqs. for typical situations.

In the p-LTE case, it is straightforward to show that the Newton-Raphson technique (by using the maxwellians M_α as starting point) applied to KE coincides with the analytical expansion and iterative calculation from CHEB (see CC) for LTE situations.

There are two possibilities for the application of NR to the p-LTE case. The first is to consider KE eqs. only for thermal particles and assume as given the distribution functions of non-thermal particles and photons (f_β). We will use here the second approach of solving the KE eqs. for all the particles and photons, assuming as known, the LHM of all those equations.

As a starting point we take as given the set of functions M_α for the thermal species, as well as some distribution functions f_β for the other species (including photons). The latter functions are supposed to satisfy their respective KE eqs. with the given M_α.

We first obtain the distribution function f^i up to iteration i (equivalent to order i in the CHEB expansion) and then the next correction δf^i is computed by linearizing the RHM again.

$$O\ f_A^i - \xi_A^i = \frac{\partial \xi_A^i}{\partial f_A}\,\delta f_A^i + \frac{\partial \xi_A^i}{\partial f_B}\,\delta f_B^i = \Lambda^i \delta f^i \qquad (32)$$

where a summation over all kind of particles or photons B is implied and ξ_A is the RHM of the KE eqs, and Λ is a matrix operator. By inverting these equations one can calculate the functions δf^i and $f^{i+1} = f^i + \delta f^i$.

The first iteration in the former procedure shows a solution for δf^i which is a linear function of the thermodynamic forces (in the following TF). We mention that due to the enormous complication of the CHEB analytical equations, at present they have only been applied to first order (equivalent to our first iteration). In contrast, the present numerical technique can easily be applied to higher orders leading to functions δf (and hence $\vec{V}_\alpha$, $\bar{\bar{\Gamma}}_\alpha$, and $\vec{q}_\alpha$) which are non linear functions of the TF and the derivatives of the TF.

Also, in the first iteration, the elastic collisions between thermal particles cancel in ξ_A^1 (but not in the derivatives), and it contains only the terms due to inelastic collisions between thermal particles and all collisions with non-thermal particles and photons. From the chosen starting point, $Of_\beta^o - \xi_\beta^o = 0$, and the f_β and then the $\xi_A{}^o$ can be expressed as functions of $Of_\beta{}^o$.

The thermodynamic forces are in principle derivatives (or logarithmic derivatives) of the thermodynamic parameters and the functions f_β with respect to the space and time variables, and the fields ($\vec{g}$, $\vec{E}$, and $\vec{B}$). However, they can be combined or expressed in terms of any independent set of variables.

In order to obtain better numerical behavior it is useful to take advantage on the isotropy of the functions M_α. As we will show, this leads to some simplification in the first iteration. We suggest in consequence to split all distribution functions f_α and f_β in symmetric and antisymmetric parts with respect to the direction of each spatial coordinate, a direction that in each case will be designated as the z axis.

If considering then, the domain of μ restricted to the interval (0,1), we have

$$f(+\mu) = (f^s(\mu) + f^a(\mu)) ,$$

and

$$f(-\mu) = (f^s(\mu) - f^a(\mu)) ,$$

The KE equations become

$$O^a f^s + O^s f^a = \xi^a$$
$$(33)$$
and $O^s f^s + O^a f^a = \xi^s$,

where the operator O is defined as before,

$$O^a = \beta\mu\frac{\partial}{\partial z} + \frac{F_z{}^s}{c}\frac{\partial}{\partial p_z} + \frac{F_x{}^a}{c}\frac{\partial}{\partial p_x} + \frac{F_y{}^a}{c}\frac{\partial}{\partial p_y}$$

$$O^s = \frac{1}{c}\frac{\partial}{\partial t} + \beta n_x\frac{\partial}{\partial_x} + \beta n_y\frac{\partial}{\partial_y} + \frac{F_z{}^a}{c}\frac{\partial}{\partial p_z} + \frac{F_x{}^s}{c}\frac{\partial}{\partial p_x} + \frac{F_y{}^s}{c}\frac{\partial}{\partial p_y} .$$

It is evident that the terms for the gravitational acceleration and the electric field forces are symmetric since they do not depend on particle velocity. On the other hand, the magnetic field force gives complicated expressions, while the component along z of its antisymmetric part vanishes

$$F_x{}^s = mg_x + ZeE_x + \frac{P_yB_z}{mc\gamma}; \qquad F_x{}^a = -\frac{P_zB_y}{mc\gamma};$$

$$F_y{}^s = mg_y + ZeE_y - \frac{P_xB_z}{mc\gamma}; \qquad F_y{}^a = \frac{P_zB_x}{mc\gamma}; \qquad (34)$$

$$F_z^{\,s} = mg_z + Z_eE_z + \frac{P_xB_y - P_yB_x}{mc\gamma}; \qquad F_z^{\,a} = 0.$$

At this point, we apply NR to solve eqs. (33), we find

$$O^af^{is} + O^sf^{ia} = \xi^{ia} + \Lambda^{is}\ \delta f^{ia} + \Lambda^{ia}\ \delta f^{is}$$

$$\text{and} \quad O^sf^{is} + O^af^{ia} = \xi^{is} + \Lambda^{ia}\ \delta f^{ia} + \Lambda^{is}\ \delta f^{is}, \tag{35}$$

where the matrices Λ are defined by the derivatives $(\frac{\partial \xi_A}{\partial f})$ as before. We remark that the corrections apply also for the non-thermal particles, since their corresponding KE eqs. are affected by δf_α to some extent, resulting in f_β functions which are slightly different from $f_\beta^{\,o}$ (the functions which satisfy the zero order KE eqs).

Equations (35) can be solved numerically by using a partition of the impulse space and expressing numerically the derivatives with respect to velocity and angles as well as the integrals over impulse space.

The equations become greatly simplified in the first iteration, since for the fluid rest frame ($\vec{U} = 0$),

$$\frac{\partial M_\alpha}{\partial P_i} = -\frac{P_i}{m\beta T} M_\alpha$$

$$\frac{\partial M_\alpha}{\partial x_i} = M_\alpha\left[\frac{\partial \ln(n_\alpha)}{\partial x_i} + \left(\frac{p^2}{2m\beta T} - \frac{d\ln K}{d\ln T}\right)\frac{\partial \ln T}{\partial x_i} - \frac{P_j}{m\beta T}\frac{\partial P_j'}{\partial U_j'}\frac{\partial U_j}{\partial x_i}\right] \tag{36}$$

$\vec{P}'$ being the impulse of the particle in an arbitrary reference frame with velocity $\vec{U}'$.

Eqs. (35) become

$$
\begin{aligned}
O^{a}M_{\alpha} &= \xi^{a}_{\alpha} + \Lambda^{s}_{\alpha}\,\delta f^{a} + \Lambda^{a}_{\alpha}\,\delta f^{s} \\
O^{s}M_{\alpha} &= \xi^{s}_{\alpha} + \Lambda^{a}_{\alpha}\,\delta f^{a} + \Lambda^{s}_{\alpha}\,\delta f^{s} \\
0 &= 0 + \Lambda^{s}_{\beta}\,\delta f^{a} + \Lambda^{a}_{\beta}\,\delta f^{s} \\
0 &= 0 + \Lambda^{a}_{\beta}\,\delta f^{a} + \Lambda^{s}_{\beta}\,\delta f^{a}.
\end{aligned}
\qquad (37)
$$

VI. The Stationary Plane Parallel Case

We will consider the simple case when all gradients of TP and all the fields ($\vec{g}$, $\vec{E}$, $\vec{B}$) are directed along the z axis and all derivatives with respect to time are zero.

Following eqs. (37), we have

$$O^a M_\alpha = \beta\mu M_\alpha\left[\frac{\partial \ln(n_\alpha)}{\partial z} + \left(\frac{mc^2\beta^2}{2kT} - \frac{3}{2}\right) + \frac{\partial \ln T}{\partial z}\right] - \frac{\beta N}{kT} M_\alpha F_z{}^s$$

$$O^s M_\alpha = \frac{mc\beta^2}{kT}\,\mu^2 M_\alpha\,\frac{\partial U_z}{\partial z}\ .$$

In these equations one can recognize the classical thermodynamic forces

$$
\begin{aligned}
X_{n_\alpha} &= \frac{\partial \ln(n_\alpha)}{\partial z} \\
X_T &= \frac{\partial \ln T}{\partial z} \\
X_z &= \frac{g_z}{c^2} \\
X_E &= \frac{E_z}{e} \\
X_U &= \frac{1}{c}\,\frac{\partial U_z}{\partial z}
\end{aligned}
\qquad (39)
$$

and the associated functions

$$Q^a_{n_\alpha} = \beta\mu M_\alpha$$

$$Q_T^a = \beta\mu\left(\frac{mc^2\beta^2}{2kT} - \frac{3}{2}\right)M_\alpha$$

$$Q_g^a = -\beta\mu \frac{mc}{kT}^2 M_\alpha$$

$$Q_E^a = -\beta\mu \frac{ze^2}{kT} M_\alpha$$

$$Q_U^s = \beta^2\mu^2 \frac{mc^2}{kT} M_\alpha .$$

Then, one can associate to each force a pair of functions δf_b^a, δf_b^s which result from the solution of the equations

$$Q_b^a X_b = \Lambda^s \delta f_b^a + \Lambda^a \delta f_b^s$$

$$0 = \Lambda^a \delta f_b^a + \Lambda^s \delta f_b^s ,$$

or (40)

$$0 = \Lambda^s \delta f_b^a + \Lambda^a \delta_b^s$$

$$Q_b^s X_b = \Lambda^a \delta f_b^a + \Lambda^s \delta f_b^s ,$$

plus the corresponding equations for non-thermal particles and photons. The last equations can be eliminated by using them to calculate the δf_β values as functions of δf_α and then replacing δf_β in the eqs. for thermal particles.

If one performs numerically the integrals which define the transport phenomena in the hydrodynamic equations, it is possible to define the weights W corresponding to the transport variables as

$$V_\alpha = W^a_\alpha \, \delta f^a$$

$$q = W^a_q \, \delta f^a \qquad (41)$$

$$\Gamma_{zz} = W^s_\Gamma \, \delta f^s,$$

and, one can define the transport coefficients Ω_{ab} by one of the following expressions

$$\Omega_{ab} = W^a_a \, (\Lambda^s - \Lambda^a \Lambda^{s^{-1}} \Lambda^a)^{-1} \, Q^a_b$$

$$\Omega_{ab} = W^a_a \, (\Lambda^a - \Lambda^s \Lambda^{a^{-1}} \Lambda^s)^{-1} \, Q^s_b$$

$$\Omega_{ab} = W^s_a (\Lambda^s - \Lambda^a \Lambda^{s^{-1}} \Lambda^a)^{-1} \, Q^s_b \qquad (42)$$

$$\Omega_{ab} = W^s_a (\Lambda^a - \Lambda^s \Lambda^{a^{-1}} \Lambda^s)^{-1} \, Q^a_b,$$

a being the index related to the flux considered, and b the index related to the thermodynamic force involved.

The present method shows a numerical way of calculating these classical transport coefficients. Moreover, it shows how to define and calculate some new coefficients which appear due to the interaction of thermal particles with non-thermal particles and with photons.

Let us consider the photons, and to be consistent with the actual situation assume that their distribution function f_ν depends only on z and μ.

We will assume they interact with particles through Boltzmann type binary collisions, hence

$$\mu \frac{\partial f_\nu^s}{\partial z} = \eta_\nu^a - \chi_\nu^s f_\nu^a - \chi_\nu^a f_\nu^s$$

$$\text{and} \quad \mu \frac{\partial f_\nu^a}{\partial z} = \eta_\nu^s - \chi_\nu^a f_\nu^a - \chi_\nu^s f_\nu^s . \tag{43}$$

For simplicity we consider a gas in which there are not non-thermal species, since at *zero order* the coefficients x_ν and η_ν are symmetric; it results

$$\mu \frac{\partial f^{os}}{\partial z} = - \chi_\nu^s f_\nu^{oa}$$

$$\mu \frac{\partial f_\nu^{oa}}{\partial z} = \eta_\nu^s - \chi_\nu^s f_\nu^{os} , \tag{44}$$

which is the Feautrier form of the radiative transfer equations.

In principle, by using eqs. (44) all the f_ν^{oa} and f_ν^{os} functions can be expressed as functions of some thermodynamic forces, which we define as

$$X_{1\nu} = \frac{\partial \ln f_\nu^{os}}{\partial z}$$

$$X_{2\nu} = \frac{\partial \ln f_\nu^{oa}}{\partial z}$$

where

$$f_\nu^{\,oa} = -\frac{\mu}{\chi_\nu^s} f_\nu^{os} X_{1\nu},$$

and $$f_\nu^{os} = \frac{n_\nu^s}{\chi_\nu^s} - \frac{\mu}{\chi_\nu^s} f^{oa} X_{2\nu}.$$

One general characteristic of the equations for thermal particles is seen directly in the present context, viz. ξ^{oa} depends only on $X_{1\nu}$ since all initial distribution functions are symmetric, except that for the photons. Moreover, since only one-photon processes are considered, that term is linear in $X_{1\nu}$ and can be expressed as

$$\xi^{oa} = \chi_A^s \; f_\nu^{oa} = - \mu\frac{\chi_A^s}{\chi_\nu^s} \; f_\nu^{os} \; X_{1\nu} \; , \tag{46}$$

χ_A^s being some coefficient dependent on the M_α.

This leads to the definition of the transport coefficients associated with the radiation flux, according to

$$\Omega_{a1\nu} = W_a^a(\Lambda^s - \Lambda^a\Lambda^{s-1}\Lambda^a)^{-1} \; Q_{1\nu}^a$$

with (47)

$$Q_{1\nu}^a = \mu\frac{\chi_A^s}{\chi_\nu^s} \; f_\nu^{os}$$

(a simple expression for χ_A^s can be obtained from $\frac{\partial \xi_A}{\partial f_\nu}$).

To analyze the coefficients associated with the force $X_{2\nu}$, one can assume that the inelastic collision term can be written as

$$\xi_A^{os} = - \eta_A^s + \chi_A^s \, f_\nu^{os},$$

where η_A^s and χ_A^s are coefficients depending on M_α.

From this, we have

$$\xi_A^{os} = - \mu\frac{\chi_A^s}{\chi_\nu^s} \, f_\nu^{oa} \, X_{2\nu} + \chi_A^s\left(\frac{\eta_\nu^s}{\chi_\nu^s} - \frac{\eta_A^s}{\chi_A^s}\right). \qquad (48)$$

The last equation gives the definition of two sets of coefficients, one associated with the force $X_{2\nu}$

$$\Omega_{a2\nu} = W_a^s(\Lambda^s - \Lambda^a \Lambda^{s^{-1}} \Lambda^a)^{-1} \, Q_{2\nu}^s$$
$$Q_{2\nu}^s = \mu\frac{\chi_A^s}{\chi_\nu^s} \, f_\nu^{oa}, \qquad (49)$$

and the second set associated with a third radiation force

$$X_{3\nu} = \chi_\alpha^s\left(\frac{\eta_\alpha^s}{\chi_\alpha^s} - \frac{\eta_\nu^s}{\chi_\nu^s}\right), \qquad (50)$$

where η_α^s and χ_α^s are the values of η_A^s and χ_A^s integrated over the impulse space. The corresponding Q is

$$Q^s_{3\nu} = \frac{\chi^s_A}{\chi^s_\alpha} \frac{\left[\dfrac{\eta^s_A}{\chi^s_A} - \dfrac{\eta^s_\nu}{\chi^s_\nu}\right]}{\left[\dfrac{\eta^s_\alpha}{\chi^s_\alpha} - \dfrac{\eta^s_\nu}{\chi^s_\nu}\right]}$$

Considering the case where the elastic collision terms are much larger than the inelastic ones, and using eqs. (40), we can distinguish between two types of forces, those for which the associated Q is antisymmetric and those for which Q is symmetric. The analysis shows that for antisymmetric forces the correction δf^s is of higher order than δf^a, and the opposite holds for the symmetric forces. Following these considerations, one can write

$$\begin{aligned} \Omega_{\alpha b} &= W^a_\alpha \, {\Lambda^s}^{-1} \, Q^a_b \\ \Omega_{qb} &= W^a_q \, {\Lambda^s}^{-1} \, Q^a_b \\ \Omega_{\Gamma b} &= W^s_\Gamma \, {\Lambda^s}^{-1} \, Q^s_b, \end{aligned} \qquad (51)$$

and then, up to the first iteration the diffusion velocities and thermal conductive flux can be expressed as the summation of the product of some transport coefficients by the antisymmetric thermodynamic forces, and the stress tensor becomes linear in the symmetric thermodynamic forces.

VII. Conclusions

We have presented the system of kinetic equations for a gas of particles and photons taking into account different forms of the collision terms.

From these equations we developed the hydrodynamic equations for the particles in a non-relativistic case without making assumptions regarding the distribution functions. These equations contain the fluxes of particles and particle impulses and energies in some linear and non-linear terms.

The latter equations are useful in any situation, in LTE and p-LTE by making the equations to be solved simpler and even in the non-LTE case for checking the accurracy and consistency of the results obtained by numerical methods.

We described a numerical method for calculating the departure from maxwellian of the distribution function of the thermal particles in the p-LTE situation (the solution obtained also applies to LTE), and show that to first order it is linear in certain thermodynamic forces which we defined.

From this departure one can calculate numerically the fluxes previously mentioned and then the transport coefficients we defined. These coefficients can be combined and compared with those defined by CC. They can also be used straightforwardly to calculate the fluxes of particles and thermal energy.

From the present expressions some coefficients are defined which are new in astrophysics although well known in other areas of physics, namely those which describe the effects of radiation or non-thermal particles on thermal particles.

Furthermore, one obtains the detailed shape of the first order departure from maxwellian f and one is able to perform the next iteration (for given values of the thermodynamic forces) obtaining $f^{(2)}$.

By comparing δf_α with M_α and δf_β with f_β one can check the validity of the hypothesis regarding the smallness of the departures and then the range of validity of the transport coefficients.

As an example we show in Figs 1 and 2 the values computed for $f/(M\mu X)$ for some simple model gases, fully ionized hydrogen (Fig. 1), and rigid spheres (Fig. 2) under some thermodynamic forces.

In these figs. one sees that for a given value of X, at some velocity (dependent upon the value of X) δf_α becomes comparable with M_α. Consequently, for velocities greater than a certain critical value (β_c), the first order approach does not hold and important departures from maxwellian can be expected, i.e. those particles with velocities greater than β_c must be considered as non-thermal particles. If the value of β_c is large enough ($\beta_c >> \beta_T = (\frac{mc^2}{2kT})^{-1/2}$), most of the particles are thermal and the high velocity particles form the so called non-thermal tail of the distribution.

The last case can be treated as a p-LTE case, but even when the non-thermal tail contains few particles, they are very energetic and can produce important effects (for instance in the ionization of some elements as was shown by Rousell-Dupree, 1980).

In another paper we will publish results already obtained by applying the present method to a partially ionized hydrogen gas, accounting for radiation in the Lyman continum.

The inclusion of important magnetic fields (those which can affect the transport coefficients) requires a careful consideration of all the collision terms in the presence of the curved trajectories of charged particles, and seems to be a very important but difficult topic, especially for partially ionized gases.

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FIGURE CAPTIONS

Fig. 1a. The departure from maxwellian ($\delta f^a/\mu M$) of the electrons (full line) and protons (dashed line) distribution functions in a gas composed by electrons and protons, for unit logarithmic gradient of the pressure ($X_P = 1\ cm^{-1}$).

Fig. 1b. The same as Fig. 1a but for unit logarithmic gradient of the temperature (at constant pressure) ($X_T = 1\ cm^{-1}$). The dash-dot line shows the SH results

Fig. 1c. The same as Fig. 1b but for unit electric force ($X_E = 1\ cm^{-1}$).

Fig. 1d. The same as Fig. 1a but for unit radiation force ($X_W = 1\ cm^{-1}$) assuming radiation of wavelength between 912 A and 304 A of mean intensity $J_\nu = WB_\nu\ (T_R)$ (B_ν being the Planck function). The values were taken as W = 1, T_R = 10,000 K, and the logarithmic gradient of W equal $1\ cm^{-1}$.

Fig. 2a. The departure from maxwellian ($\delta f^a/\mu M$) in a gas composed by rigid spheres for unit logarithmic gradient of the pressure ($X_P = 1\ cm^{-1}$).

Fig. 2b. The same as Fig. 2a but for unit logarithmic gradient of the temperature (assuming constant pressure) ($X_T = 1\ cm^{-1}$).